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Methane Opacities in T Dwarf Atmospheres

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Abstract. We present the current status of PHOENIX model atmospheres for dwarfs of the spectral type T, typical for older field brown dwarfs and low-mass brown dwarfs. The results are based on new predictions of the CH₄ line opacities from theoretical calculations with the STDS software package, extrapolating to transitions from rotational levels up to $J = 40$. While individual line positions and strengths are reproduced with moderate to fair accuracy, the cumulative band strength in the region of the IR methane bands is modelled much better thanks to the inclusion of large numbers of faint lines relevant at high temperatures.

1. Methane Dwarfs

The transition between spectral classes L and T, as T_{eff} drops below ~ 1300 K, is characterised by a reduction of the effects of dust absorption and the appearance of CH₄ absorption bands in the infrared, showing up in the coolest brown dwarfs which have only recently been discovered in substantial numbers in the field. These features appearing in the K and, from spectral type T0, in the H band and growing in strength with decreasing temperature, are one of the basic characteristics defined in the classification schemes of Geballe et al. (2002) and Burgasser et al. (2002) for the T spectral class. As one of the dominant opacity sources in these objects besides H₂O and CIA H₂, the CH₄ molecular bands are also of great importance for the correct modelling of ultracool substellar atmospheres and for evolutionary calculations of old brown dwarfs.

2. Line Opacity Predictions

A major problem in model atmosphere calculations for substellar objects is the paucity of molecular opacity data for the temperature regime of brown dwarfs. Available line lists from spectroscopic databases for Earth and planetary atmospheres, based on both experimental data and theoretical predictions, are com-

piled for much lower temperatures and thus often lack transitions from lower states at higher energies.

Theoretical approaches to model the energy levels and transition probabilities of CH₄ are challenged by the complexity of the vibrational systems (polyads) of the molecule, due to resonances of the four vibrational modes. This leads to eight vibrational bands with 24 subbands already in the third system (Octad) and 14 bands/60 subbands in the fourth (Tetradecad).

The Spherical Top Data System (STDS) (Wenger & Champion 1998) based on the tetrahedral formalism allows simulations of the line systems up to the Tetradecad. Subsequent analyses of experimental data over the past decade have significantly improved the input parameters for the predictions of the polyads up to the Octad (Hilico et al. 2001). We have used the 2001 version of the STDS software to calculate line opacity predictions for all available systems, extrapolating up to upper-state rotational levels of $J = 40$.

Table 1. STDS line statistics vs. 1996 HITRAN and GEISA data.

Transition	J_{\max}	$\lambda[\mu\text{m}]$	Number of lines
GS \rightarrow GS	40	22.2 – 10 ⁶	5470
GS \rightarrow P1	40	4.59 – 15.7	57 441
GS \rightarrow P2	40	2.56 – 5.80	218 243
GS \rightarrow P3	40	1.77 – 3.58	631 728
GS \rightarrow P4	40	1.35 – 2.59	1 608 020
P1 \rightarrow [P1 – P4]	25	1.79 – 10 ⁶	1 178 216
P2 \rightarrow [P2 – P4]	20	2.39 – 10 ⁶	6 593 824
HITRAN	10 ?	1.6 – 100	30 049
GEISA	?	5.0 – 10	6659

3. Model Spectra

Atmosphere models using the new opacity data have been computed with PHOENIX version 12, with other opacity sources included as prescribed in the AMES-cond grid (Allard et al. 2001). The dust opacities are treated in the limit of complete settling, thus describing the complete removal of all grains from the photosphere. We have tested the models on the recent observations of Geballe et al. (2002) and present here comparisons with the spectrum of the T 4.5 brown dwarf SDSS 0207+00, taken at $\sim 10 \text{ \AA}$ resolution with NIRCAM/Keck II.

The original AMES-Cond models show a clear lack of opacity in these regions, particularly on the blue sides of the bands. Comparison of the K-band spectra with a preliminary model including levels up to $J \leq 20$ illustrate the improvement achieved by the additional levels in the Octad system, but only the line list including at least levels up to $J \leq 30$ gives a good fit over the full band shape.

The H band features are more difficult to reproduce with the STDS predictions, since this wavelength region is dominated by transitions to the Tetradecad and higher vibrational levels. The current STDS version only includes parame-

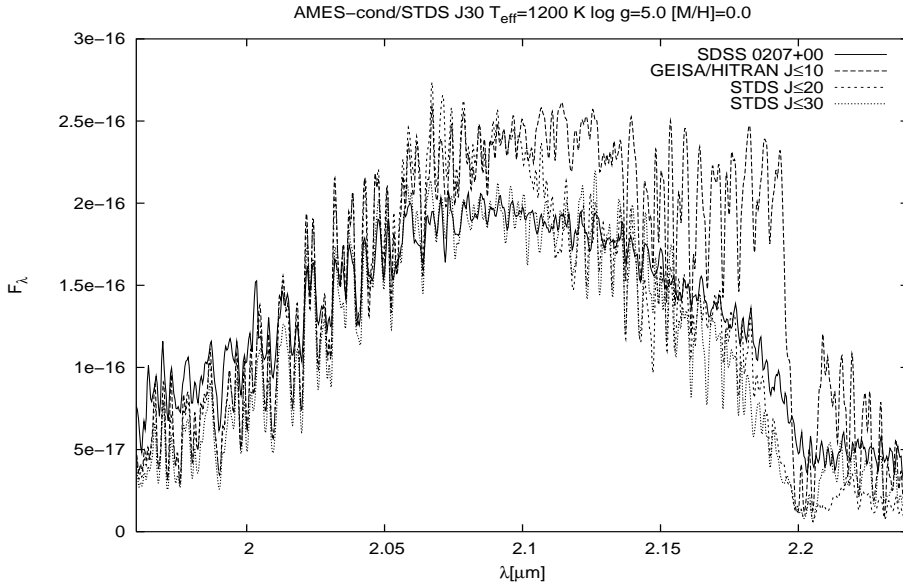


Figure 1. Comparison of the K band spectra for the original AMES-cond model and models using the STDS line opacity predictions to an observed T dwarf spectrum. The new models include GS-Octad transitions computed up to J of 20 and 30, respectively.

ters for the TetradeCAD extrapolated from the analysis of lower polyad systems, which resulted in a lack of opacity at many wavelengths. Newer calculations using preliminary results from the analysis of the TetradeCAD system (V. Boudon 2002, *priv. comm.*) show considerable improvement over the earlier versions, although individual line strengths are still not very well reproduced.

All models still tend to overestimate the absorption in the regions of strongest opacity, for both CH_4 and H_2O bands. This is probably due to errors in the atmospheric temperature structure of the current models describing only the limiting case of full dust condensation. This problem will be addressed by a self-consistent model for gravitational settling of grains (Allard et al., *in prep.*).

4. Hot Bands

Inclusion of hot bands, transitions originating from higher polyads, was limited by the upper polyads STDS can handle. Thus for the K-band only an extrapolation for the TetradeCAD-Dyad was available, while in the H-band region no hot bands could be computed at all. Although the upper polyads are sparsely populated at T dwarf temperatures, due to the steeply increasing degeneracy their cumulative strength can still contribute a significant background opacity which might only be treated in a statistical approach (Borysow et al., these proceedings). These limitations in the hot band models result in an uncertainty in the total absorption strength that is comparable in effect to an uncertainty in T_{eff} of ~ 100 K or 0.5 dex in $\log g$ and metallicity.

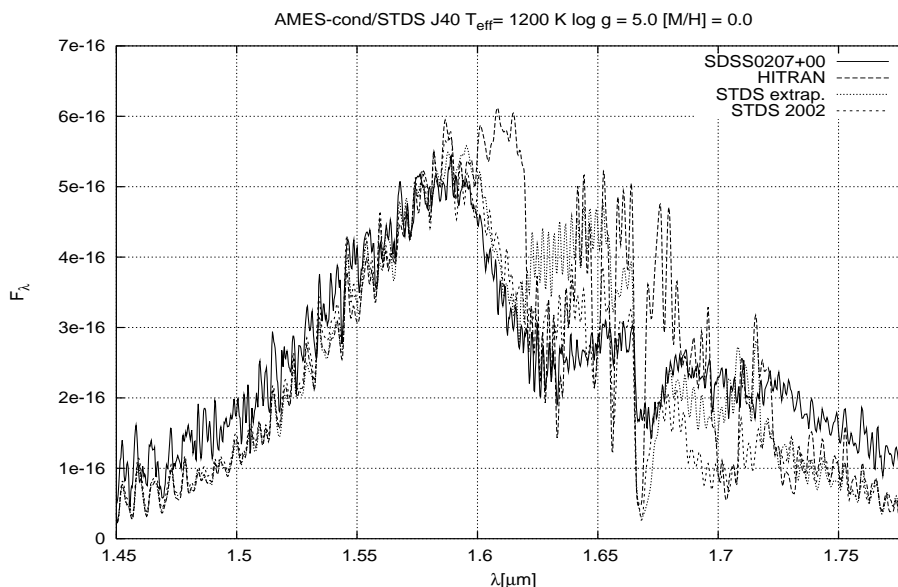


Figure 2. H band spectra for AMES-cond model and two STDS models using extrapolated data from the Octad, and preliminary results from the Tetradecad analysis.

5. Conclusions

STDS-created line lists produce opacity data that significantly improve on the HITRAN and GEISA databases and allow a much more detailed analysis of the IR spectra and comparison with observationally derived spectral indices for brown dwarfs. With respect to the contribution of higher polyads several uncertainties remain that could affect the quantitative determination of atmospheric parameters based on molecular absorption features. A realistic description of the atmospheric structure will also require a more sophisticated treatment of dust formation which is currently under way.

5.1. Acknowledgements

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